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On the Relation of Modulated Structures with the Automorphisms of the *d*-Dimensional Tori Created by the Compaction of the (3+*d*)-Dimensional Space

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Abstract

A hypothesis is put forward concerning the existence of the general relation between aperiodic crystal structures and the invariants of the group of the automorphisms of the d-dimensional torus. A relation is proved between the one-dimensional and two-dimensional displacive modulations and the rationality of some invariants of the group of automorphisms of both the circle S^1 and the torus T^2.

1. Introduction

Incommensurately (IC) modulated crystal structures do not possess translational symmetry in three-dimensional space, whereas in commensurately (C) modulated crystal structures one can always redefine the basic vectors of the crystal lattice in such a way that the translational symmetry is restored in three dimensions. As a result of this operation, the volume of the elementary cell of the basic structure always increases. IC modulation is characterized by the fact that both the modulation vectors and the basic vectors of the reciprocal lattice are linearly independent over the field of rational numbers. This means that in IC structures the translational symmetry breaks and they cannot be described by the three-dimensional crystallographic symmetry space groups. The symmetry of such systems is described by the superspace groups (*e.g.* Janner *et al.*, 1983), which are defined in (3+d)-dimensional space, where d is the number of the modulation vectors in the elementary cell of the crystal lattice.

The incommensurability of the crystal structure served as a necessary condition for the application of the superspace groups to the description of the modulated structures at the first stage of development of de Wolff's idea of the supercrystal (de Wolff, 1974). However, it turned out in the mathematical derivation of the superspace groups (Janssen & Janner, 1979) that the incommensurability condition was not essential so superspace groups can also be applied to the descriptions of commensurate structures. In general, the position of the jth atom in the nth elementary cell of the displacively modulated structure is given by

$$\mathbf{r}(j, \mathbf{n}) = \mathbf{n} + \mathbf{r}_j + \mathbf{u}(j, \mathbf{n}), \tag{1}$$

where $\mathbf{n} = (n_1, n_2, n_3)$ and n_1, n_2, n_3 are integers; vector $\mathbf{n}$ is defined with respect to an arbitrary (but fixed) basis. $\mathbf{r}_j$ is the position of this atom in the $\mathbf{n}$th elementary cell of the basic (nonmodulated) structure and $\mathbf{u}$ is a periodic displacive modulation function defined with respect to the same basis as $\mathbf{n}$. Thus, one can say that the modulated structure can be described by both the basic structure $\mathbf{r}_j$ and the displacement field $\mathbf{u}$.

To introduce the idea of a supercrystal, one has to define the superspace in which a modulated structure regains the translational symmetry. Superspace V_S is a simple sum of the real space R^3 and a certain vector space V_d:

$$V_S = R^3 \oplus V_d. \tag{2}$$

V_d is a d-dimensional space.

In the $(n+d)$-dimensional space V_S, an Euclidean group of motions $E(n+d)$ acts, which is a semisimple product of the orthogonal group $O(n+d)$ and translational group $T(n+d)$. The superspace group Γ_S is a subgroup of the group $E(n+d)$ satisfying the conditions

$$\begin{array}{ll} \text{(i)} & \Gamma_S \cap T(n+d) \simeq Z^{n+d} \\ \text{(ii)} & \Gamma_S \cap T(d) \simeq Z^d, \end{array} \tag{3}$$

where $T(d)$ is a translational group in V_d.

Condition (i) says that in V_S there exists a lattice Σ, which is invariant with respect to $T(n+d)$:

$$T(n+d)\Sigma = \Sigma.$$

Condition (ii) says that in V_d there exists a lattice D, which is invariant with respect to $T(d)$:

$$T(d)D = D.$$

In such a case, the translational subgroup $T(d)$ is isomorphic with Z^d.

One can now modify equation (1) to make possible the description of atoms in V_S. After such a modification, one obtains the following formula for the displacively modulated structures:

$$\mathbf{r}(j, \mathbf{n}, \mathbf{t}) = \mathbf{n} + \mathbf{r}_j + \mathbf{u}_j(\mathbf{q} \cdot \mathbf{n} + \mathbf{q}_d \cdot \mathbf{t}), \tag{4}$$

where $\mathbf{n}, \mathbf{q} \in R^3$; $\mathbf{t}, \mathbf{q}_d \in V_d$, $\mathbf{q}$ being the modulation

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vector in R^3 and $\mathbf{q}_d$ being the corresponding vector in V_d.

Let us connect with every atom in physical space a surface in V_S, which is described by a vector parameter $\mathbf{t}$. This surface, called the atomic surface $F_{j\mathbf{n}}$, is defined as

$$F_{j\mathbf{n}} = \{(\mathbf{r}, \mathbf{t}) \in V_S | r_\alpha = r_\alpha(j, \mathbf{n}, \mathbf{t}), \alpha = 1, 2, 3\}, \quad (5)$$

r_α being components of the vector (4) in the R^3 space.

For each pair $(j, \mathbf{n})$ and $(j', \mathbf{n}')$, the two corresponding atomic surfaces $F_{j\mathbf{n}}$ and $F_{j'\mathbf{n}'}$ are topologically equivalent with each other and with respect to the space V_d. The family of all the atomic surfaces $F_{j\mathbf{n}}$ is called the family F:

$$F = \{F_{j\mathbf{n}}\}. \quad (6)$$

All the surfaces $F_{j\mathbf{n}}$ are infinite surfaces. However, as they are topologically equivalent to V_d, one can compact them because in V_d there acts transitively a translation group $T(d)$ isomorphic with the set of integers Z^d and retaining the lattice D. The compaction consists here in the creation of the quotient structure:

$$V_d/Z^d \simeq F/Z^d \simeq T^d, \quad (7)$$

T^d being a d-dimensional torus.

The aim of this work is to study a relationship between the modulated structures and the invariants of automorphisms S^1 (in the case of $d = 1$) and T^2 (in the case of $d = 2$) as well as to put forward a hypothesis that, depending on the d value, there can exist different aperiodic crystal structures, *e.g.* incommensurately modulated structures and quasicrystals. Both mentioned structures do not possess the translational symmetry but from different reasons: the former because of the appearance in the crystal of a periodic physical property, whose period is not commensurate with the corresponding lattice period; the latter because of the appearance in the crystal of a symmetry element that is not consistent with any of the three-dimensional space groups (see *e.g.* Janot, 1994). Let us assume that in all cases of aperiodicity here both main and satellite reflections are sharp, which corresponds to the long-range interaction.

To realise the aim mentioned above, an analysis of the group of automorphisms of the d-dimensional T^d is carried out.

2. Modulated structure in the (3+*d*)-dimensional space (where *d* = 1, 2) and the number of rotations

Let us assume the simplest case of the displacive modulation, *i.e.* for $d = 1$. Then T^1 is a one-dimensional circle S^1. The modulation function $\mathbf{u}(\tau)$ has the following form:

$$u_i(\tau) = \sum_{n=-\infty}^{+\infty} u_{in} \exp(2\pi i n \tau), \quad (8)$$

where $i = 1, 2, 3$ and u_i are the coordinates of $\mathbf{u}$ with respect to the same basis as (1). The function $\mathbf{u}(\tau)$ is defined on the circle S^1 with the values in R^3. For each i $(= 1, 2, 3)$, u_i defines a mapping of S^1 into R^1:

$$u_i : S^1 \to R^1. \quad (9)$$

With the aid of u_i, one can define the map φ_i, which transforms S^1 into S^1:

$$\varphi_i(\tau) = \tau + u_i(\tau). \quad (10)$$

In other words, we defined the mapping Φ from the set of functions on S^1 with the values in R^1 $[\mathcal{F}(S^1, R^1)]$ into the set of automorphisms S^1 $[\mathrm{Aut}(S^1)]$, which can be written as

$$\Phi : \mathcal{F}(S^1, R^1) \to \mathrm{Aut}(S^1).$$

In our case [see (10)],

$$\Phi(u_i(\tau)) = \varphi_i(\tau).$$

To prove that φ_i maps S^1 into S^1, notice that

$$\varphi_i(\tau + 1) = \varphi_i(\tau) + 1 \quad (11)$$

and that two points p_1 and p_2 on the circle are equivalent if

$$p_1 - p_2 = 2\pi n, \quad n \text{ integer}. \quad (12)$$

The maps $\varphi_i(\tau)$ are the automorphisms S^1.

Having a modulated structure in $R^3 \oplus R^1$, one can pass to $R^3 \oplus S^1$ according to the *Introduction*. The physical condition assumed at such a transition is that the type of modulation should not change, *i.e.* if we deal with the IC structure then after the transition the IC structure remains. This condition says that the same type of modulation should remain at the arbitrary continuous map of S^1 into S^1. In other words, the type of modulation should be invariant of the group of automorphisms S^1. It turns out that the number of rotations ρ, which was first introduced by Denjoy (1932), makes such an invariant. Let us recall its definition and the corresponding theorems (Coddington & Levinson, 1955).

Let φ be the map of S^1 into S^1. Let us denote $\varphi^n \equiv \varphi \circ \ldots \circ \varphi$ (n times), which presents the n-fold composition of the map φ. The point τ is the periodic point of the type m/n if

$$\varphi^n(\tau) = \tau + m, \quad (13)$$

where $m, n \in Z$. The number of rotations ρ of the map φ is defined as

$$\lim_{n\to\infty} \varphi^n(\tau)/n = \rho. \quad (14)$$

The theorems concerning the periodic points and the number of rotations are the following:

Theorem 1. (Coddington & Levinson, 1955.) For each $\tau_0 \in S^1$, there exists

$$\lim_{n\to\infty} \varphi^n(\tau_0)/n = \rho$$

and it does not depend on the point τ_0. The number ρ is rational when and only when φ has a periodic point.

Theorem 2. (Godbillon, 1983.) Let $\psi = \omega \circ \varphi \circ \omega^{-1}$, where ω is a homeomorphism S^1 into S^1 and $\varphi, \psi : S^1 \to S^1$, then:

(a) $\rho_\varphi = \rho_\psi$, if ω keeps the orientation of S^1;

(b) $\rho_\varphi + \rho_\psi = 0$, if ω changes the orientation of S^1.

As follows from Theorem 2, ρ is an invariant with respect to the group of automorphisms S^1. We can now apply the above definitions and theorems to the case under study. Let us fix one of the components of the modulation function (8) and let us denote it as $u(\tau)$. For the other components, our considerations will be analogous. According to the above definition, one can link with the modulation function $u(\tau)$ the number of rotations ρ:

$$\rho = \lim_{n\to\infty} \varphi_u^n(\tau)/n, \qquad (15)$$

where

$$\varphi_u(\tau) = u(\tau) + \tau. \qquad (16)$$

The invariance of ρ with respect to the group of automorphisms S^1 agrees with our physical condition that the type of modulation cannot change at the maps of the circle S^1 into S^1. Our invariant ρ is a well defined quantity, which can serve for the classification of the structures with a single modulation.

Let us assume that $\varphi_u(\tau)$ possesses a periodic point, which means that the number of rotations ρ is rational. One can now state the following theorem:

Theorem 3. If ρ is rational, then the modulated structure is commensurate.

Proof. Assume that our modulated structure be described with the aid of the modulation function $\mathbf{u}$ [equation (8)]. (We fix, as above, one of the components of u.) The physical condition says that the type of modulation cannot change at any automorphism S^1. Let us choose now a map ν_N:

$$\nu_N : S^1 \to S^1 \qquad (17)$$

in the form

$$\nu_N(\tau) = \varphi_u^N(\tau)/N. \qquad (18)$$

Putting together u and ν_N, one obtains

$$u(\nu_N(\tau)) = \sum_{n=0}^{+\infty} u_n \exp[2\pi i n \nu_N(\tau)] \equiv u'(\tau). \qquad (19)$$

$u'(\tau)$ is a new modulation function and, in particular when $N \to \infty$, the type of modulation should not change:

$$\lim_{N\to\infty} u(\nu_N(\tau)) = \lim_{N\to\infty} \sum_{n=0}^{+\infty} u_n \exp[2\pi i n \nu_N(\tau)] = \sum_{n=0}^{+\infty} u_n \exp(2\pi i n \rho), \qquad (20)$$

where ρ is the number of rotations [see (14)]. We have assumed in the above equation that (a) the function u is continuous and (b) the series defining u is uniformly convergent.

Assuming that ρ is a rational number of the form

$$\rho = q/p, \qquad (21)$$

we can now write the last expression in (20) as

$$S = \sum_{n=0}^{+\infty} u_n \exp(2\pi i n q/p). \qquad (22)$$

The above sum can be rewritten as follows:

$$S = \sum_{n=0}^{p-1} u_n(p) \exp(2\pi i n q/p), \qquad (23)$$

where

$$u_n(p) = \sum_{n=0}^{+\infty} u_{kp+n}. \qquad (24)$$

Thus, if ρ is a rational number, then the sum in (20) is a finite sum, which corresponds to the commensurate modulation function and proves Theorem 3. Note that, as follows from equations (4), (8), (10), (14), (15), (18)–(24), the number of rotations ρ is rational only when the modulation parameter (ratio of the absolute value of the modulation wavevector and the proper reciprocal-lattice period) is rational. For the same reasons, if the number of rotations ρ is irrational then the modulation parameter is also irrational and corresponds to an incommensurate modulation.

The essence of Theorem 3 is a construction of mapping Φ from the class of modulated structures M (in the case of one-dimensional modulation) into a group of automorphisms S^1 [Aut(S^1)] and then finding such a mapping of group Aut(S^1) into real numbers R^1, which allows us to distinguish the inequivalent elements of Aut (S^1). We say that f and f' are equivalent (belong to the same class) if there exists an $\omega \in$ Aut(S^1) such that

$$f' = \omega \circ f \circ \omega^{-1}, \qquad (25)$$

where $f, f' \in$ Aut(S^1).

As it turns out, the number of rotations ρ makes such a mapping (see Theorem 2). In our case, the mapping Φ transforms a modulation function into an element of Aut(S^1) and has the following form:

$$\Phi(u(\tau)) \equiv u(\tau) + \tau = \varphi(\tau). \qquad (26)$$

In this formalism, Theorem 3 has a new form:

Theorem 3′. If $\rho(\varphi) \in Q$, then M is commensurate, where

$$\rho\,(\text{number of rotations}) : \mathrm{Aut}(S^1) \to R^1, \quad Q \text{ is the set of rational numbers.} \tag{27}$$

Carrying out identical reasoning for each of the components of the modulation function (8), one can conclude that, if all the numbers of rotations, *i.e.* ρ_1, ρ_2 and ρ_3, related to the coordinates $u_1(\tau)$, $u_2(\tau)$ and $u_3(\tau)$, respectively, are rational, then the structure is commensurate.

The above formalism can be generalized for the case when the space V_d has dimension d higher than 1. In such a case, Φ is a mapping from the class of aperiodic structures A into a group of automorphisms of the d-dimensional torus [$\mathrm{Aut}(T^d)$]:

$$\Phi : A \to \mathrm{Aut}(T^d). \tag{28}$$

Let us define a mapping ρ_i ($i = 1, \ldots, K$; K is the number of invariants) of the group $\mathrm{Aut}(T^d)$ into a class of the real numbers R^1:

$$\rho_i : \mathrm{Aut}(T^d) \to R^1. \tag{29}$$

One can then say that f and f', being elements of $\mathrm{Aut}(T^d)$, belong to the same class if

$$\rho_i(f) = \rho_i(f') \tag{30}$$

for all $i = 1, \ldots, K$ (number of invariants).

One can then put forward a hypothesis: *The number of inequivalent aperiodic structures is equal to the number of classes of $\mathrm{Aut}(T^d)$ defined by $\{\rho_1 \ldots \rho_K\}$.* If we carried out similar reasoning for the atomic surfaces F, we would cope with the two difficulties:

(i) If g and g' map F into F, which means that $g, g' : F \to F$ or, in other words, $g, g' \in \mathrm{Aut}\,(F)$ then the same automorphism f belonging to $\mathrm{Aut}(T^d)$ will correspond to g and g' when

$$g' = g + h, \tag{31}$$

where $h \in \mathrm{GL}(d, Z)$.

It is because, according to the construction of T^d as the quotient space F/Z^d, two points x and $x' \in F$ are considered identical on the torus T^d when $x' = x + v$, where $v \in Z^d$. Let us assume that $g(x) = y$ and $g'(x) = y'$. Then $g'(x)$ and $g(x)$ correspond to the same point on the torus when

$$g'(x) = g(x) + w, \quad w \in Z^d. \tag{32}$$

If we take another vector $w' \in Z^d$, then the above relation will also take place. In general, let $h : Z^d \to Z^d$, then

$$g'(x) = g(x) + hw \tag{33}$$

$$[w \in Z^d \quad \text{and} \quad h \in \mathrm{GL}(d, Z)].$$

Thus,

$$\mathrm{Aut}(T^d) = \mathrm{Aut}(F) \bmod \mathrm{GL}(d, Z). \tag{34}$$

One can then see that to the one automorphism $f \in \mathrm{Aut}\,T^d$ the whole family of automorphisms F corresponds, which is parametrized with the elements of the group $\mathrm{GL}(d, Z)$. If one considers the group $\mathrm{Aut}(F)$, then the problem arises with the unequivocal choice of $g \in \mathrm{Aut}(F)$. This inconvenience disappears only when we are on the torus T^d (after the compaction).

(ii) In consequence of the ambiguity of the choice of $g \in \mathrm{Aut}(F)$, one should construct invariants $\chi_i : \mathrm{Aut}(F) \to R^1$, which would result in the same value for the arguments g and g' related by $g' = g + h$:

$$\chi_i(g + h) = \chi_i(g), \quad h \in \mathrm{GL}(d, Z). \tag{35}$$

The above formula says that the domain of χ_i is the group of automorphisms T^d, thus $\chi_i = \rho_i$, where

$$\rho_i : \mathrm{Aut}(T^d) \to R^1. \tag{36}$$

To illustrate what was said above, let us assume the displacive modulation and $d = 2$. In this case, an atomic surface is given by

$$F_2 = \{(t_1, t_2, u_1(t_1, t_2), u_2(t_1, t_2), u_3(t_1, t_2)) \in R^5 \mid t_1, t_2 \in R^1\} \subset R^5 \tag{37}$$

(F_2 is a two-dimensional surface in R^5). Each of the functions $u_i(\mathbf{t})$ is periodic in t_1 and t_2:

$$u_i(t_1 + m_1, t_2 + m_2) = u_i(t_1, t_2), \tag{38}$$

where $m_1, m_2 \in Z$.

If one identifies points $t_1 + m_1$ with t_1 and $t_2 + m_2$ with t_2, then F_2 becomes a two-dimensional torus T^2 in R^5. It follows from the fact that two points belonging to R^5, namely

$$p = (t_1, t_2, u_1(\mathbf{t}), u_2(\mathbf{t}), u_3(\mathbf{t})) \tag{39a}$$

and

$$p' = (t_1 + m_1, t_2 + m_2, u_1(\mathbf{t}), u_2(\mathbf{t}), u_3(\mathbf{t})), \tag{39b}$$

are equivalent because

$$p' - p = (m_1, m_2, 0, 0, 0). \tag{40}$$

Compaction here means identifying the points with the coordinates $(t_1 + m_1, t_2 + m_2)$ with the points with the coordinates (t_1, t_2). So, after compaction, the atomic surface F_2 becomes a two-dimensional torus T^2 in R^5, as mentioned before. Let us denote the group of automorphisms of the two-dimensional torus as $\mathrm{Aut}(T^2)$. If $\varphi \in \mathrm{Aut}(T^2)$, then

$$\varphi : T^2 \to T^2$$
$$\varphi(\mathbf{t}) = (\varphi_1(\mathbf{t}), \varphi_2(\mathbf{t})). \quad (41)$$

One can link two invariants with the automorphism φ (analogously to the case when φ: $S^1 \to S^1$):

$$\rho_1 = \lim \varphi_1^n(\mathbf{t})/n \quad n \to \infty \quad (42a)$$
$$\rho_2 = \lim \varphi_2^n(\mathbf{t})/n \quad n \to \infty, \quad (42b)$$

where the n-fold composition $\varphi^n = \varphi \circ \ldots \circ \varphi$ is defined as

$$\varphi^n(\mathbf{t}) = (\varphi_1(\varphi^{n-1}(\mathbf{t})), \varphi_2(\varphi^{n-1}(\mathbf{t}))). \quad (43)$$

Let us take one of the components of the modulation function [see (38)] and denote it as

$$u(t_1, t_2) = \sum_{k,l} u_{kl} \exp[2\pi i(kt_1 + lt_2)]. \quad (44)$$

This function maps T^2 into R^1.

One can link with the function u an automorphism of the torus T^2 in the following way:

$$\varphi(\mathbf{t}) = (u(\mathbf{t}) + t_1, u(\mathbf{t}) + t_2). \quad (45)$$

The character of the function u should not change under the action of the automorphism φ acting on u in the following way:

$$u(\varphi(\mathbf{t})) = \sum_{k,l} u_{kl} \exp\{2\pi i[\varphi_1(\mathbf{t})k + \varphi_2(\mathbf{t})l]\}. \quad (46)$$

The composition of φ^n/n with the function u has the form

$$u(\varphi^n(\mathbf{t})/n) = \sum u_{kl} \exp\{2\pi i[k/n\varphi^n(\mathbf{t}) + l/n\varphi^n(\mathbf{t})]\}. \quad (47)$$

Passing with n to ∞, one obtains

$$u(\rho_1, \rho_2) = \sum_{k,l} u_{k,l} \exp[2\pi i(k\rho_1 + l\rho_2)]. \quad (48)$$

One can distinguish three cases:

(i) ρ_1 and ρ_2 are rational, which means

$$\rho_1 = p_1/q_1, \quad \rho_2 = p_2/q_2. \quad (49)$$

In such a case, the series $u(\rho_1, \rho_2)$ assumes the form

$$u(\rho_1, \rho_2) = \sum_{n=0}^{q_1-1} \sum_{m=0}^{q_2-1} u_{n,m}(q_1, q_2) \times \exp[2\pi i(np_1/q_1 + mp_2/q_2)], \quad (50)$$

where

$$u_{n,m}(q_1, q_2) = \sum_{k,l} u_{kq_1+n,lq_2+m}. \quad (51)$$

So this case corresponds to the commensurate modulation.

(ii)

$$\rho_1 = p/q \text{ (rational)}, \quad \rho_2 \text{ irrational}. \quad (52)$$

In this case,

$$u(\rho_1, \rho_2) = \sum_{k=0}^{q-1} \sum_{l} u_{n,l}(q) \exp[2\pi i(np/q + l\rho_2)] \quad (53)$$

and

$$u_{n,l}(q) = \sum_{k} u_{kq+n,l}. \quad (54)$$

It corresponds to the case when the two-dimensional modulation reduces to the incommensurate modulation in one direction and to the commensurate modulation in the other direction. This reasoning contains also the case when ρ_1 is irrational and ρ_2 is rational. It follows from the fact that the additional dimensions of the superspace V_S are indistinguishable.

(iii) ρ_1 and ρ_2 are irrational. Then the modulation is incommensurate.

Thus, in the case of $d = 1$, one has only two inequivalent classes: commensurate and incommensurate structures and one mapping ρ_i (number of rotations), where $i = 1$, which means that $K = 1$.

For $d \geq 2$, the number K of invariants ρ_i increases. Note that the same type of reasoning can be applied also to those quasicrystals that can be described in terms of a basic structure and a modulation, but the proper type of the modulation function should be used in (8) and (44).

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